X-Ray Standing Wave Measurements of the Gd_2O_3 / GaAs(001) Interface

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Beamline(s): **X15A**

We examine the interfacial Gd atomic structure of strained Gd_2O_3 films grown epitaxially on GaAs(001) using fluorescence-yield X-ray standing waves.

Thin Gd_2O_3 films have gained technological interest as a possible stable, passivating surface oxide for GaAs. At Bell Laboratories, Lucent Technologies, the two Gd_2O_3 films studied were grown epitaxially on GaAs(001) substrate wafers and capped with amorphous Si in ultrahigh vacuum. The samples were determined to be 3 and 6 Gd-O layers thick (layer spacing = $\sqrt{2}$ a / 8 = 1.92 Å) by comparing the Gd Lα fluorescence peak areas with a third sample determined to be 8 Gd-O layers thick by X-ray diffraction.

X-ray Standing Wave (XSW) experiments were performed at beamline X15A at the NSLS. The reflected beam intensity and the Gd Lα fluorescence yield were monitored as the scattering angle was moved through the (004), (202), and (022) Bragg reflections of GaAs. The incident x-ray energies were hν = 10.05 keV for the (004) reflection and hν = 9.50 keV for the (202) and (022) reflections. The Bragg scattering was in the vertical plane.

Figures 1 and 2 show the Gd Lα fluorescence yield XSW data for the 3 layer thick Gd_2O_3 film for the (004) and (022) reflections of GaAs, respectively. The coherent position D and coherent fraction F are determined from fitting the lineshapes to the standard XSW equation. These two quantities correspond to the phase and amplitude of the X-ray structure factor for the position distribution of the Gd atoms only.

From the (004) reflection XSW data, which measures the position distribution normal to the surface, we find D = 0.034 ± 0.008 and F = 0.219 ± 0.009 on the 3 Gd-O layer thick sample, while the thicker 6-layer sample gives D = 0.006 ± 0.007 and F = 0.152 ± 0.005. The low coherent fraction in both cases results from destructive interference between the multiple atomic layers of Gd_2O_3 .

The (202) and (022) reflections have in-surface components which provide information about the interface registry of Gd atoms. The coherent positions and fractions for the two reflections are very similar, with D = 0.480 ± 0.003 and F = 0.350 ± 0.005 for the (202) reflection and D = 0.488 ± 0.003 and F = 0.375 ± 0.005 for the (022) reflection. This in-plane symmetry is consistent with our strain model developed for a 23Å Gd_2O_3 film on GaAs(001) using EXAFS measurements (Nelson et al., Appl. Phys. Lett. **76,** 2526 (2000)).

If the strained Gd_2O_3 film in this model were placed on the GaAs(001) surface without any atomic rearrangement at the interface, the coherent fractions for the (202) and (022) reflections would vanish, due to equal population of three possible Gd sites. Preferential vacancy of one of these sites, or large displacements of Gd atoms at the interface, would result in incomplete destructive interference and is consistent with the measured nonzero coherent fraction. The proposed vacancy also agrees with electron counting arguments for the interfacial bonds.

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References: E. J. Nelson et al., Appl. Phys. Lett. **76,** 2526 (2000); M. Hong et al., Science **283**, 1897 (1999); A.R. Kortan et al., Phys. Rev. B **60**, 10913.

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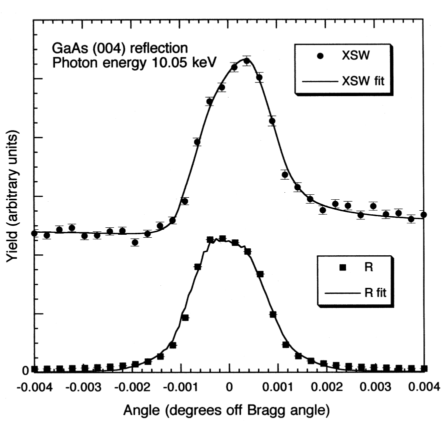

Figure 1. Gd Lα fluorescence XSW yield and reflectivity as a function of scattering angle for the (004) reflection of GaAs.

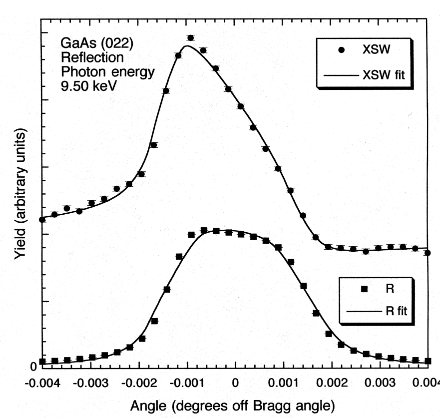

Figure 2. Gd Lα fluorescence XSW yield and reflectivity as a function of scattering angle for the (022) reflection of GaAs